

SECTION 4: SUBSEQUENT TASKS AND STUDIES

The results of the dissolver cold-flow modelling studies conducted in the 2- and 5-in.-i.d. Plexiglas columns have been summarized in this report. These initial studies became the basis for additional programs in three-phase flow hydrodynamics in support of the SRC-I Demonstration Plant dissolver design. The following is a list of these programs, abstracted from "R&D Summary Final Reports" (13), giving their numbers, titles, objectives, and conclusions:

12.1.2: Large-Scale Dissolver Cold-Flow Modelling

Objectives

- o Summarize all cold-flow work completed at ICRC that relates to the dissolver modelling.
- o Study the impact of the data acquired on SRC-I Demonstration Plant scale-up.

Abstract

The effect of liquid and gas velocities and column diameter on the axial dispersion coefficient and on solids distribution was studied. Similarly, the effect of physical properties of liquids on gas holdup, solids distribution, and liquid/gas mass transfer was examined. The liquids tested were tetralin, water, and a 50% glycol/water mixture. Gas and liquid velocities ranged from 0.05-0.4 ft/sec and from 0.01-0.05 ft/sec, respectively,

Conclusions

- o Gas holdup is not affected by column diameter size.
- o Increasing surface tension decreases holdup.
- o Liquid superficial velocity does not affect holdup.
- o Gas holdup can be affected by pressure.
- o Gas superficial velocity affects holdup and the axial liquid dispersion coefficient.
- o Internals do not affect holdup, the axial liquid dispersion coefficient, or the gas/liquid mass transfer coefficient.
- o Gas spargers increase gas holdup and the gas/liquid mass transfer coefficient.
- o Solids axial distribution is affected by particle size concentration, liquid physical properties, and liquid superficial velocity.
- o Gas velocity variations do not affect solids axial distribution if the gas velocity is above the critical velocity.
- o The gas/liquid mass transfer is not the limiting step in the hydrogenation of coal.
- o The use of internals in the dissolver, such as distributor or target plates, is not beneficial.
- o Cold-flow data are in line with the scale-up effort for the Baseline design of the dissolver.

12.1.3: Effect of Dissolver Solids and Solvent IBP on Dissolver Performance

Objectives

- o Quantify the extent to which the mineral-rich solids, which accumulate in the dissolver of the Wilsonville Advanced Coal Liquefaction Facility, catalyze coal liquefaction reactions.
- o Determine the effect of process solvent IBP on the net product yield.

Abstract

Mineral-rich reaction residues, filter cake, and Kerr-McGee ash concentrate (KMAC) were added to the feed of the bench-scale SRC-I dissolver to simulate the performance of the dissolver solids. Filter cake catalyzes the preasphaltene conversion and solvent hydrogenation reactions, indicating that dissolver solids are catalytically active. The impact of varying solvent IBP on product yields was also studied.

Conclusions

- o Filter cake, and presumably dissolver solids, catalyze the preasphaltene conversion and solvent hydrogenation reactions.
- o These materials do not catalyze asphaltene conversion or increase hydrocarbon gas yield.
- o This catalytic activity results from the specific minerals contained in filter cake/dissolver solids rather than from a general increase in surface area.

- o The unconverted coal and SRC in filter cake and KMAC residues are reactive at SRC-1 dissolver conditions.
- o Therefore, recycle of these residues increases net coal conversion and the combined yield of oil plus asphaltenes, while reducing preasphaltene yield.
- o The improvements in product slate are achieved without increasing hydrocarbon gas yield.
- o The residues do not significantly promote solvent hydrogenation in the absence of coal.
- o The initial boiling point of the process solvent does not significantly affect product yield.

12.1.5: Impact of Hydrodynamics on Coal Liquefaction

Objectives

- o Develop a laboratory-scale tubular reactor system to study process parameters that cannot be determined by a continuous stirred tank reactor (CSTR) alone.
- o Determine the impact of reactor hydrodynamics on coal liquefaction.
- o Expand the data base to assist in kinetic model development.

Abstract

The R&D data base generated to support the SRC-1 plant design has been essentially based on data from the CSTR and on hydrodynamic studies from cold-flow simulation. In order to study the hydrodynamic impact more directly, a

bench-scale tubular reactor was developed that performed coal liquefaction in the plug flow fluid dynamic regime. The design basis for the plug flow reactor was developed from an extensive cold-flow study and a computer simulation of coal liquefaction at various reactor configurations. The effect of reactor hydrodynamics on product distribution was determined from the results obtained from both a CSTR and the plug flow reactor. Kentucky #9 Mulford coal was used for this study. The existing sequential model was tested against both data bases.

Conclusions

- o Design of a plug flow reactor required thorough characterization of the flow behavior in order to ensure that the reactor actually operated in the plug flow regime.
- o The plug flow reactor had a significant advantage over the CSTR reactor, increasing coal conversion by 6%, preasphaltene conversion by 10%, and oil yield by 10%. However, these improved yields were less than those predicted by the sequential model.
- o Both CSTR and plug flow data are desirable to assist in developing an appropriate process reaction model.

12.1.7: Effects of Accumulated Solids and Staged Vessels on Dissolver Performance

Objectives

- o Determine the effect on conversion, yield structure, solvent rehydrogenation, and desulfurization of adding inert solids to the reaction slurry.
- o Determine the effect of operating the dissolvers in series and parallel modes.
- o Determine conversion, yield, and hydrogen consumption after the first dissolver in a simulated series operation.
- o Expand the data base to both 20- and 60-min residence times.
- o Show the effect of operating at low hydrogen feed rates.

Abstract

A once-through process run was conducted in which 10 wt % finely divided quartz was added to the feed slurry of the bench-scale SRC-I dissolver to study the effect of inert solids on yield structure. An additional reactor was installed in the coal process development unit (CPDU) to study the effect of series vs. parallel operation of the dissolvers. The effect of staged temperature operation of the two dissolvers on yield distribution was also examined. Finally, the effect of time and temperature on yield distribution was studied with a high-reactive coal.

Conclusions

- o Inert material does not catalyze hydrogenation reactions; merely increasing the available surface area does not alter the yield distribution.

- o Operating the dissolvers in series decreases the yield of preasphaltenes. Neither conversion nor oil, asphaltene, or gas yield is affected by reactor configuration.
- o Oil yields increase with an increase in residence time, but are insensitive to changes in temperature.
- o Coal conversion is insensitive to changes in residence time and temperature (in the range of 20 to 60 min and 780 to 840°F).
- o Hydrocarbon gas yield and hydrogen consumption increase with an increase in temperature and residence time.
- o Qualitatively, the data tend to support a series reaction mechanism.
- o The staged temperature operation of the dissolvers may have some potential advantages. Oil yields are improved by operating the first reactor at a lower temperature than the second one. Hydrocarbon gas yields and hydrogen consumption are lower in the staged temperature mode than in an isothermal mode.
- o The partitioning of hydrogen between the front end of the reaction train and the second dissolver may have a detrimental effect on product yields.